

n-Hexane  
110-54-3 | DTXSID0021917

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 131 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.93e-01

Confidence level: 8.30e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Bromopentane</div> <div>Measured: 151</div> <div>Predicted: 7.15</div>	<div>Image not found</div> <div>3,6-Diacetylmorphine</div> <div>Measured: 82.7</div> <div>Predicted: 1.04e-09</div>	<div>Image not found</div> <div>1-Chloropropene</div> <div>Measured: 105</div> <div>Predicted: 345</div>
<div>Image not found</div> <div>1,3,5-Trifluorobenzene</div> <div>Measured: 57.8</div> <div>Predicted: 91.1</div>	<div>Image not found</div> <div>2-Methylpyrazine</div> <div>Measured: 514</div> <div>Predicted: 1.86</div>	